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Molecular Dynamics Conference **(Statement A)**
(San Diego, CA, 18-20 May 2003) (Deadline: 08 Apr 2003)

Polynitrogen Chemistry

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Under combined DARPA, AFOSR, NSF, and DOE sponsorship, we have continued our work in polynitrogen chemistry. We have successfully prepared and characterized numerous polyazido compounds, such as $As(N_3)_3$, $Sb(N_3)_3$, $As(N_3)_5$, $Sb(N_3)_5$, $As(N_3)_6^-$, $Sb(N_3)_6^-$, $Te(N_3)_4$, $Te(N_3)_6^{2-}$, $P(N_3)_6^-$, and $B(N_3)_4^-$, and have studied the combination of N_5^+ with some of these anions. Most of these compounds are extremely energetic and shock sensitive.

We have studied the reactions of the NF_4^+ and $N_2F_3^+$ cations with HN_3 in HF solution. The synthesis of the N_7^- anion was also pursued by preparing and characterizing R_3SiNCl_2 and $(R_3Si)_2NCl$ compounds. Although their chlorine atoms could not be replaced by azido groups, the reaction of the latter with HF/MF_5 resulted in the isolation of salts of the novel monochloroammonium cation.

Enthalpies of formation were calculated for gas phase N_3, N_3^-, N_5^+, and N_5^- from *ab initio* molecular orbital theory. Stability calculations were carried out for solid $N_5^+N_3^-$ and $N_5^+N_5^-$, using these values and lattice energy estimates.

The possible existence of FN_5 was studied both experimentally by FT-IR spectroscopy of the volatile decomposition products from the thermolysis of $(N_5^+)_2SnF_6^{2-}$ and computationally using a RRKM analysis.